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Molecular dynamics studies of impulse driven reactions in molecules and molecular clusters

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Synopsis We have used molecular dynamics methods to study collisions between atoms and molecules or molecular clusters. We find that these collisions may yield highly reactive molecular fragments and efficient intracluster covalent bond-forming reactions in the cluster. There is a good agreement between our simulations and various experimental results.

Recent studies have shown that collisions between atoms/ion and molecules, in the energy range of a few tens of eV to a few tens of keV, can result in fragmentation pathways not typically found when photons or electrons are used to excite molecular systems. An example of this is the knockout process, where individual atoms may be ejected from a molecule in Rutherford-like scattering processes [1]. This mechanism has also been found to result in the production of highly reactive fragments, leading to a significant reduction in barrier heights for forming covalent bonds between molecules, for example within clusters of PAH- or fullerene molecules [2, 3].

Classical and ab initio molecular dynamics simulations have played an important role in our understanding of the mechanisms that occur in collisions between atoms and isolated molecules or their clusters [2, 3, 4, 5, 6]. Overall we have found a good agreement between the simulations and the experimental results, both qualitatively and quantitatively. Examples of this include studying reaction barriers between molecules and fragments [2, 5, 6], determining reaction cross sections [3, 4], identifying molecular species that are formed in the reactions [2, 3, 5], and simulating fragment mass spectra [3].

At the conference we will present an overview of the simulation methods that we have developed as well as an update on recent results.

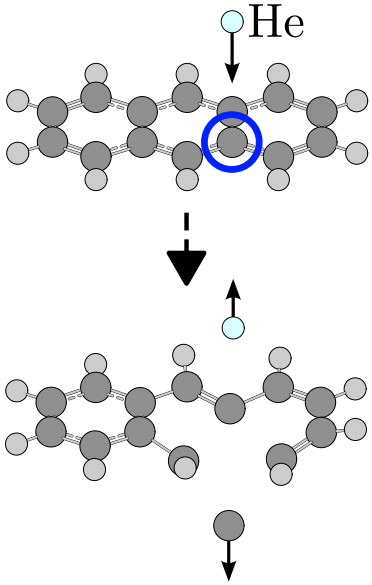

Figure 1. Two frames from a simulation of He colliding with anthracene ($C_{14}H_{10}$) where a single C-atom is knocked out from the molecule in a scattering process.

References

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